



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:21 AM UTC

PDB ID : 8K9R / pdb_00008k9r
EMDB ID : EMD-36996
Title : Cryo EM structure of the products-bound PGAP1(Bst1)-H443N from *Chaetomium thermophilum*
Authors : Li, T.; Hong, J.; Qu, Q.; Li, D.
Deposited on : 2023-08-01
Resolution : 2.68 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

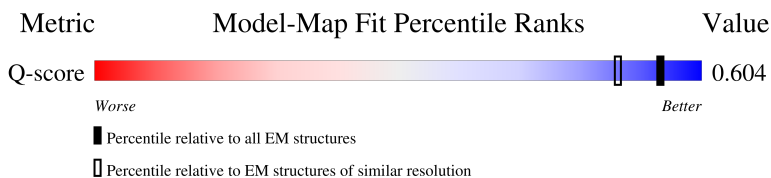
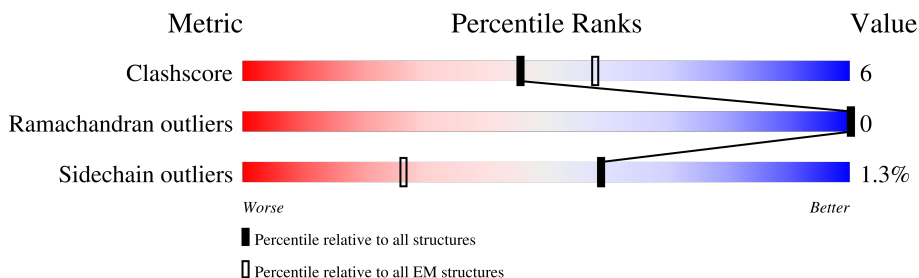
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9255 (2.18 - 3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1447	
2	B	272	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7684 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GPI inositol-deacylase,MCherry protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	958	7487	4856	1264	1334	33	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP G0S652
A	0	GLY	-	expression tag	UNP G0S652
A	1	SER	-	expression tag	UNP G0S652
A	443	ASN	HIS	engineered mutation	UNP G0S652
A	1185	GLY	-	linker	UNP G0S652
A	1186	THR	-	linker	UNP G0S652
A	1187	LEU	-	linker	UNP G0S652
A	1188	GLU	-	linker	UNP G0S652
A	1189	VAL	-	linker	UNP G0S652
A	1190	LEU	-	linker	UNP G0S652
A	1191	PHE	-	linker	UNP G0S652
A	1192	GLN	-	linker	UNP G0S652
A	1193	GLY	-	linker	UNP G0S652
A	1194	PRO	-	linker	UNP G0S652
A	1195	LYS	-	linker	UNP G0S652
A	1196	LEU	-	linker	UNP G0S652
A	1197	GLU	-	linker	UNP G0S652
A	1198	PHE	-	linker	UNP G0S652
A	1345	SER	TRP	engineered mutation	UNP A0A366VY15
A	1363	VAL	ILE	engineered mutation	UNP A0A366VY15
A	1365	TYR	GLN	engineered mutation	UNP A0A366VY15
A	1399	ARG	ILE	engineered mutation	UNP A0A366VY15
A	1434	SER	-	expression tag	UNP A0A366VY15
A	1435	ALA	-	expression tag	UNP A0A366VY15
A	1436	HIS	-	expression tag	UNP A0A366VY15
A	1437	HIS	-	expression tag	UNP A0A366VY15
A	1438	HIS	-	expression tag	UNP A0A366VY15
A	1439	HIS	-	expression tag	UNP A0A366VY15

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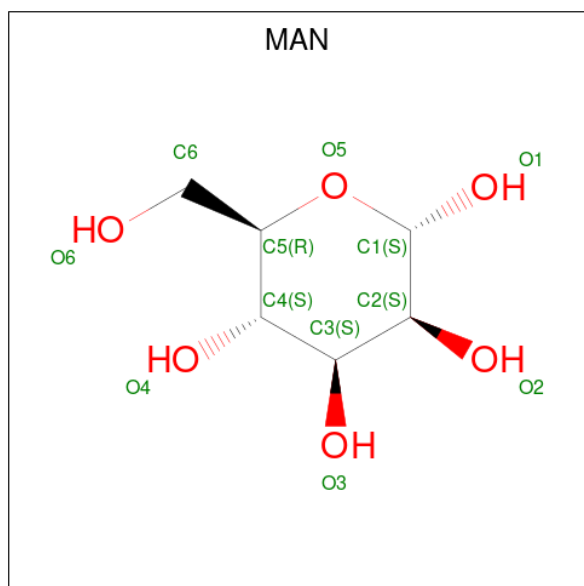
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1440	HIS	-	expression tag	UNP A0A366VY15
A	1441	HIS	-	expression tag	UNP A0A366VY15
A	1442	HIS	-	expression tag	UNP A0A366VY15
A	1443	HIS	-	expression tag	UNP A0A366VY15
A	1444	HIS	-	expression tag	UNP A0A366VY15
A	1445	HIS	-	expression tag	UNP A0A366VY15

- Molecule 2 is a protein called Green fluorescent protein, Complement decay-accelerating factor.

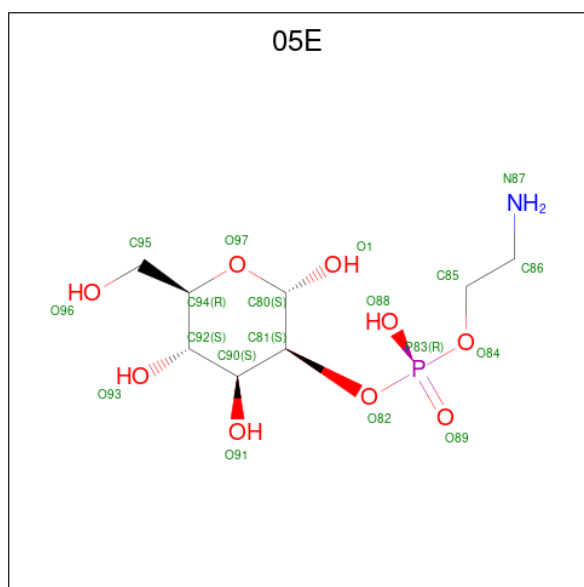
Mol	Chain	Residues	Atoms			AltConf	Trace
2	B	4	Total	C	N	O	
			24	13	4	7	
							0
							0

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



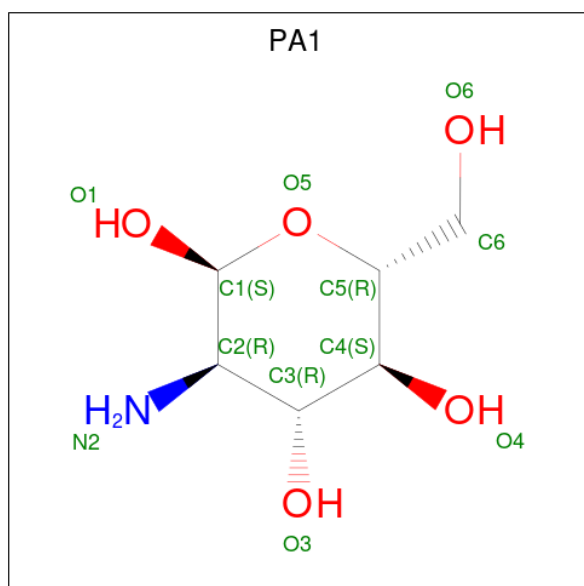
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	
			11	6	5	
						0
3	A	1	Total	C	O	
			11	6	5	
						0

- Molecule 4 is 2-azanylethyl [(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-2,4,5-tris(oxidanyl)oxan-3-yl] hydrogen phosphate (CCD ID: 05E) (formula: $C_8H_{18}NO_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			18	8	1	8	1	

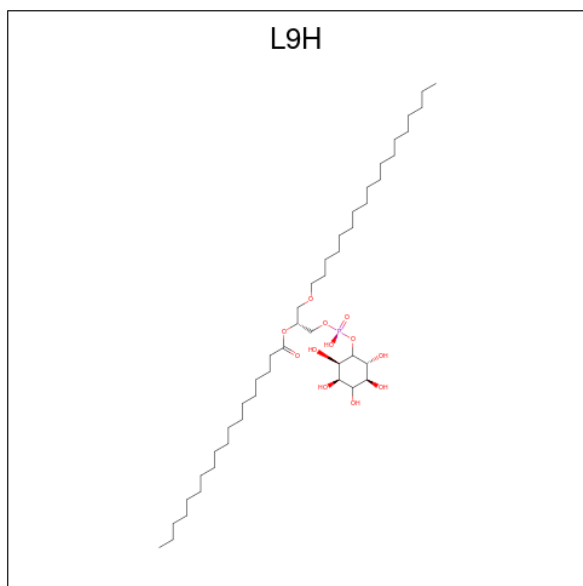
- Molecule 5 is 2-amino-2-deoxy- α -D-glucopyranose (CCD ID: PA1) (formula: $C_6H_{13}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			11	6	1	4	

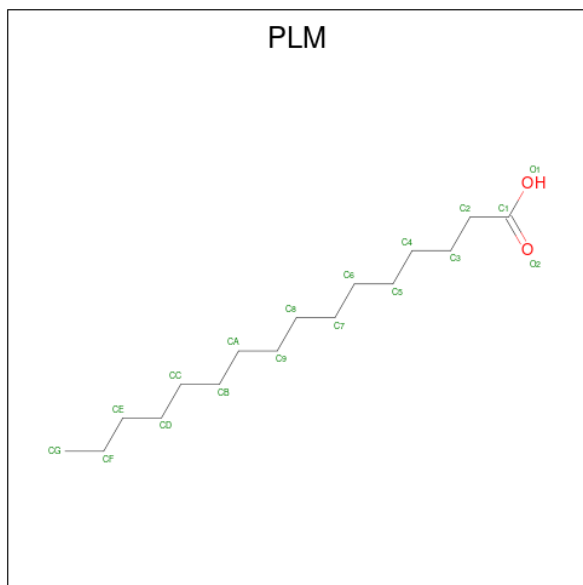
- Molecule 6 is [(2 {R})-1-octadecoxy-3-[oxidanyl-[(2 {R}),3 {R}),5 {S}),6 {R}))-2,3,4,5,6-pentakis(oxidanyl)cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] octadecanoate (CCD ID: L9H)

(formula: $C_{45}H_{89}O_{12}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			58	45	12	1	

- Molecule 7 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			18	16	2	

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			28	27	1	

- Molecule 9 is 2-azanylethyl [(2R,3S,4S,5S,6S)-3,4,5,6-tetrakis(oxidanyl)oxan-2-yl]methyl hydrogen phosphate (CCD ID: 80Y) (formula: $C_8H_{18}NO_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			18	8	1	8	1	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	179980	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.588	Depositor
Minimum map value	-2.490	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.78	Depositor
Map size (Å)	251.64, 251.64, 251.64	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, PA1, 05E, PLM, MAN, L9H, 80Y

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/7686	0.49	1/10499 (0.0%)
2	B	0.66	0/23	1.64	1/30 (3.3%)
All	All	0.41	0/7709	0.50	2/10529 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	THR	N-CA-C	-6.10	106.82	114.56
1	A	235	LYS	N-CA-C	-5.40	106.37	113.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7487	0	7480	94	0
2	B	24	0	24	2	0
3	A	22	0	19	0	0
4	A	18	0	0	0	0
5	A	11	0	10	1	0
6	A	58	0	0	0	0
7	A	18	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	28	0	46	1	0
9	B	18	0	0	0	0
All	All	7684	0	7610	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LEU:HB3	1:A:702:ARG:HD3	1.69	0.73
1:A:178:ARG:NH2	1:A:634:GLU:OE2	2.23	0.71
1:A:698:LEU:CB	1:A:702:ARG:HD3	2.22	0.69
1:A:324:LEU:HD22	1:A:351:ILE:HB	1.74	0.67
1:A:741:ARG:NH1	1:A:786:GLN:OE1	2.31	0.63
1:A:238:ARG:HB3	1:A:239:PRO:HD3	1.81	0.62
1:A:441:MET:HE1	1:A:452:PHE:HB2	1.81	0.62
1:A:1146:VAL:O	1:A:1149:THR:HG22	1.99	0.62
1:A:244:ALA:HB2	1:A:457:ILE:HD12	1.83	0.59
1:A:183:ARG:HB3	1:A:211:GLN:CD	2.28	0.59
1:A:522:ARG:NH1	1:A:671:GLU:OE2	2.35	0.58
1:A:818:THR:HA	7:A:1506:PLM:HD1	1.86	0.57
1:A:1090:MET:HE3	1:A:1091:ILE:HG22	1.86	0.57
1:A:716:SER:OG	1:A:815:ARG:NH2	2.38	0.56
1:A:334:ARG:HH22	1:A:376:ASN:HA	1.69	0.56
8:A:1507:CLR:H161	8:A:1507:CLR:H242	1.89	0.54
1:A:821:ALA:HB2	7:A:1506:PLM:HD2	1.90	0.53
1:A:285:LEU:HD12	1:A:332:VAL:HG22	1.91	0.53
1:A:509:VAL:O	1:A:602:THR:N	2.42	0.52
1:A:526:ARG:NH1	1:A:792:THR:OG1	2.41	0.52
1:A:1066:PHE:HB3	1:A:1071:ASN:OD1	2.09	0.52
1:A:213:ILE:HG21	1:A:245:ALA:HB1	1.92	0.52
1:A:281:HIS:ND1	1:A:1053:VAL:HG11	2.24	0.52
1:A:462:ASP:OD2	1:A:485:TRP:NE1	2.39	0.51
1:A:835:GLN:NE2	1:A:846:ILE:O	2.40	0.51
1:A:1117:LEU:HD13	1:A:1135:PHE:CD2	2.46	0.51
1:A:312:ASP:HB2	1:A:315:LEU:HG	1.92	0.51
1:A:678:SER:HB3	1:A:703:PRO:HG2	1.94	0.50
1:A:742:GLN:HE21	1:A:783:LEU:HD11	1.76	0.50
1:A:483:LYS:HG2	1:A:487:LEU:HD12	1.92	0.50
1:A:359:ARG:HH21	1:A:1126:VAL:HG12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:THR:HG23	1:A:475:ARG:HG2	1.94	0.49
1:A:174:PRO:HB2	1:A:627:PHE:HZ	1.77	0.49
1:A:324:LEU:CD2	1:A:351:ILE:HB	2.42	0.49
1:A:994:ILE:HD12	1:A:998:LEU:HD23	1.95	0.49
1:A:702:ARG:NH1	1:A:797:ILE:HG22	2.27	0.49
1:A:823:PHE:HD2	1:A:922:CYS:SG	2.36	0.49
1:A:326:HIS:NE2	1:A:443:ASN:O	2.45	0.49
1:A:742:GLN:NE2	1:A:783:LEU:HD11	2.28	0.48
1:A:239:PRO:O	1:A:453:ARG:HD2	2.12	0.48
1:A:185:SER:HB3	1:A:209:ARG:O	2.14	0.48
1:A:698:LEU:HB2	1:A:702:ARG:HD3	1.96	0.48
1:A:994:ILE:HG23	1:A:998:LEU:HD23	1.96	0.48
1:A:209:ARG:HA	1:A:214:ASP:OD2	2.15	0.47
1:A:699:PRO:O	1:A:702:ARG:HB2	2.14	0.47
1:A:823:PHE:O	1:A:826:PHE:HB3	2.15	0.47
1:A:490:MET:HG3	1:A:614:ILE:HD13	1.96	0.47
1:A:183:ARG:HG2	2:B:2:THR:HB	1.97	0.47
1:A:328:MET:O	1:A:332:VAL:HG23	2.15	0.46
1:A:217:VAL:O	1:A:217:VAL:HG13	2.16	0.46
1:A:744:LEU:HD11	1:A:763:LEU:HD12	1.96	0.46
1:A:168:VAL:HG23	1:A:169:THR:HG23	1.99	0.45
1:A:386:LYS:HD2	1:A:387:TRP:CZ3	2.52	0.45
1:A:183:ARG:HB2	1:A:210:GLU:OE2	2.16	0.45
1:A:282:GLY:HA3	1:A:367:GLN:HB3	1.98	0.44
1:A:238:ARG:NH1	2:B:4:SER:O	2.51	0.44
1:A:333:ALA:O	1:A:336:MET:HB2	2.17	0.44
1:A:1060:VAL:O	1:A:1061:HIS:HB2	2.18	0.44
1:A:901:ASP:O	1:A:1127:SER:OG	2.28	0.43
1:A:182:MET:HE2	1:A:239:PRO:HA	1.99	0.43
1:A:903:LEU:HB3	1:A:904:ILE:H	1.70	0.43
1:A:576:VAL:HA	1:A:604:LEU:HD23	2.00	0.43
1:A:807:GLY:O	1:A:811:LYS:HG2	2.18	0.43
1:A:823:PHE:CD2	1:A:918:ILE:HG22	2.53	0.43
1:A:496:LYS:HA	1:A:496:LYS:HD3	1.81	0.43
1:A:940:ILE:O	1:A:944:ILE:HG12	2.18	0.43
1:A:1105:LEU:O	1:A:1109:ILE:HG13	2.19	0.43
1:A:359:ARG:HH11	1:A:359:ARG:HG3	1.84	0.43
1:A:872:LEU:HD11	1:A:912:LEU:HD11	2.00	0.43
1:A:430:PHE:O	1:A:433:THR:HG22	2.19	0.43
1:A:550:LYS:NZ	1:A:674:ASP:OD1	2.45	0.43
1:A:711:PRO:HB3	1:A:781:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:O	1:A:274:ASN:ND2	2.53	0.42
1:A:704:MET:HE3	1:A:704:MET:HB3	1.74	0.42
1:A:911:PHE:HB3	1:A:914:LEU:HD12	2.00	0.42
1:A:525:LEU:O	1:A:667:PHE:HA	2.19	0.42
1:A:1094:THR:HG21	1:A:1106:LEU:HB2	2.01	0.42
1:A:327:SER:HB3	1:A:328:MET:H	1.66	0.42
1:A:431:THR:HB	1:A:441:MET:HE3	2.00	0.42
1:A:828:VAL:HG21	1:A:1042:TRP:CD1	2.55	0.42
1:A:207:LEU:HD23	1:A:217:VAL:HG23	2.02	0.41
1:A:407:ASP:OD1	1:A:443:ASN:HB2	2.21	0.41
1:A:484:LYS:HA	1:A:484:LYS:HD3	1.79	0.41
1:A:938:ARG:O	1:A:942:VAL:HG23	2.19	0.41
1:A:1007:GLN:NE2	1:A:1033:VAL:HG13	2.35	0.41
1:A:818:THR:HA	7:A:1506:PLM:CD	2.51	0.41
1:A:1075:ILE:HG23	1:A:1076:MET:HE2	2.02	0.41
1:A:177:CYS:SG	1:A:441:MET:HG2	2.61	0.41
1:A:433:THR:HB	1:A:750:SER:H	1.85	0.41
1:A:522:ARG:HG3	1:A:524:VAL:HG23	2.02	0.41
1:A:915:ILE:HB	1:A:916:PRO:HD3	2.01	0.41
1:A:231:ALA:O	5:A:1504:PA1:N2	2.54	0.40
1:A:817:ARG:O	7:A:1506:PLM:HD1	2.21	0.40
1:A:222:VAL:HG21	1:A:464:VAL:HB	2.04	0.40
1:A:996:TYR:HB2	1:A:1075:ILE:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	950/1447 (66%)	924 (97%)	26 (3%)	0	100	100
2	B	2/272 (1%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	952/1719 (55%)	926 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	822/1249 (66%)	812 (99%)	10 (1%)	63	82
2	B	3/219 (1%)	2 (67%)	1 (33%)	0	0
All	All	825/1468 (56%)	814 (99%)	11 (1%)	59	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	ARG
1	A	327	SER
1	A	620	THR
1	A	621	ARG
1	A	702	ARG
1	A	704	MET
1	A	728	GLU
1	A	903	LEU
1	A	904	ILE
1	A	906	THR
2	B	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	367	GLN
1	A	436	ASN
1	A	652	GLN

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Mol	Chain	Res	Type
1	A	701	ASN
1	A	1026	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	05E	A	1503	3,5	18,18,19	0.65	0	21,25,27	0.90	1 (4%)
9	80Y	B	101	3,2	18,18,19	0.63	0	24,25,27	0.99	1 (4%)
3	MAN	A	1501	9	11,11,12	0.43	0	15,15,17	0.81	0
8	CLR	A	1507	-	31,31,31	0.32	0	48,48,48	0.63	0
7	PLM	A	1506	-	17,17,17	0.53	0	17,17,17	0.50	0
5	PA1	A	1504	6,4	11,11,12	0.77	0	13,15,17	1.47	2 (15%)
3	MAN	A	1502	9,4	11,11,12	0.56	0	15,15,17	0.95	2 (13%)
6	L9H	A	1505	5	58,58,58	0.37	0	66,69,69	0.52	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	05E	A	1503	3,5	-	4/12/29/32	0/1/1/1
9	80Y	B	101	3,2	-	10/11/28/31	0/1/1/1
3	MAN	A	1501	9	-	0/2/19/22	1/1/1/1
8	CLR	A	1507	-	-	5/10/68/68	0/4/4/4
7	PLM	A	1506	-	-	7/15/15/15	-
5	PA1	A	1504	6,4	-	2/2/19/22	0/1/1/1
3	MAN	A	1502	9,4	-	0/2/19/22	0/1/1/1
6	L9H	A	1505	5	-	20/52/76/76	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	101	80Y	O53-C52-C85	-3.81	102.25	110.15
5	A	1504	PA1	C1-O5-C5	3.73	117.18	112.19
5	A	1504	PA1	C4-C3-C2	-2.95	106.38	111.37
6	A	1505	L9H	O10-C9-C7	-2.89	103.57	110.38
3	A	1502	MAN	O2-C2-C3	-2.37	105.25	110.15
3	A	1502	MAN	O2-C2-C1	-2.20	104.18	109.22
4	A	1503	05E	C80-O97-C94	2.14	115.05	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1503	05E	O84-C85-C86-N87
4	A	1503	05E	C85-O84-P83-O82
4	A	1503	05E	C85-O84-P83-O88
9	B	101	80Y	O72-C73-C74-O75
9	B	101	80Y	C83-C73-C74-O75
9	B	101	80Y	C74-O75-P76-O77
9	B	101	80Y	C74-O75-P76-O81
9	B	101	80Y	C74-O75-P76-O82
8	A	1507	CLR	C17-C20-C22-C23
6	A	1505	L9H	CD8-CD9-CE0-CE1
5	A	1504	PA1	O5-C5-C6-O6
6	A	1505	L9H	CD6-CD7-CD8-CD9

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Mol	Chain	Res	Type	Atoms
5	A	1504	PA1	C4-C5-C6-O6
8	A	1507	CLR	C21-C20-C22-C23
8	A	1507	CLR	C20-C22-C23-C24
6	A	1505	L9H	CB1-CB2-CB3-CB4
6	A	1505	L9H	OD1-CD2-CD3-CD4
6	A	1505	L9H	CD3-CD4-CD5-CD6
6	A	1505	L9H	CD5-CD6-CD7-CD8
6	A	1505	L9H	CB8-CB9-CC0-CC1
6	A	1505	L9H	CD7-CD8-CD9-CE0
7	A	1506	PLM	C7-C8-C9-CA
8	A	1507	CLR	C23-C24-C25-C27
6	A	1505	L9H	CE2-CE3-CE4-CE5
7	A	1506	PLM	C3-C4-C5-C6
6	A	1505	L9H	CC4-CC5-CC6-CC7
6	A	1505	L9H	CD4-CD5-CD6-CD7
6	A	1505	L9H	CC0-CC1-CC2-CC3
7	A	1506	PLM	CD-CE-CF-CG
6	A	1505	L9H	CE5-CE6-CE7-CE8
9	B	101	80Y	C73-C74-O75-P76
7	A	1506	PLM	C9-CA-CB-CC
6	A	1505	L9H	CB6-CB7-CB8-CB9
8	A	1507	CLR	C23-C24-C25-C26
6	A	1505	L9H	CE6-CE7-CE8-CE9
6	A	1505	L9H	CB4-CB5-CB6-CB7
7	A	1506	PLM	C6-C7-C8-C9
6	A	1505	L9H	OA7-CA8-CA9-CD0
6	A	1505	L9H	OA7-CA8-CA9-OB0
6	A	1505	L9H	CA9-CD0-OD1-CD2
4	A	1503	05E	C85-O84-P83-O89
9	B	101	80Y	C78-O77-P76-O75
9	B	101	80Y	C78-O77-P76-O81
9	B	101	80Y	C78-O77-P76-O82
9	B	101	80Y	O77-C78-C79-N80
6	A	1505	L9H	CC3-CC4-CC5-CC6
7	A	1506	PLM	C5-C6-C7-C8
7	A	1506	PLM	CA-CB-CC-CD

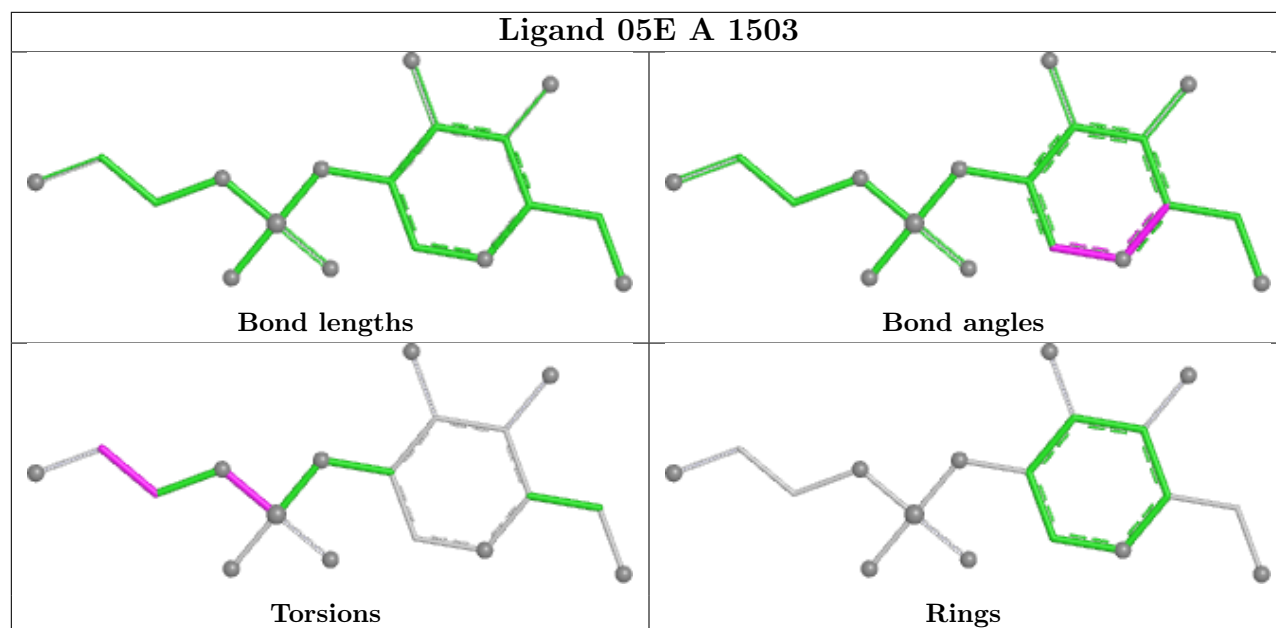
All (1) ring outliers are listed below:

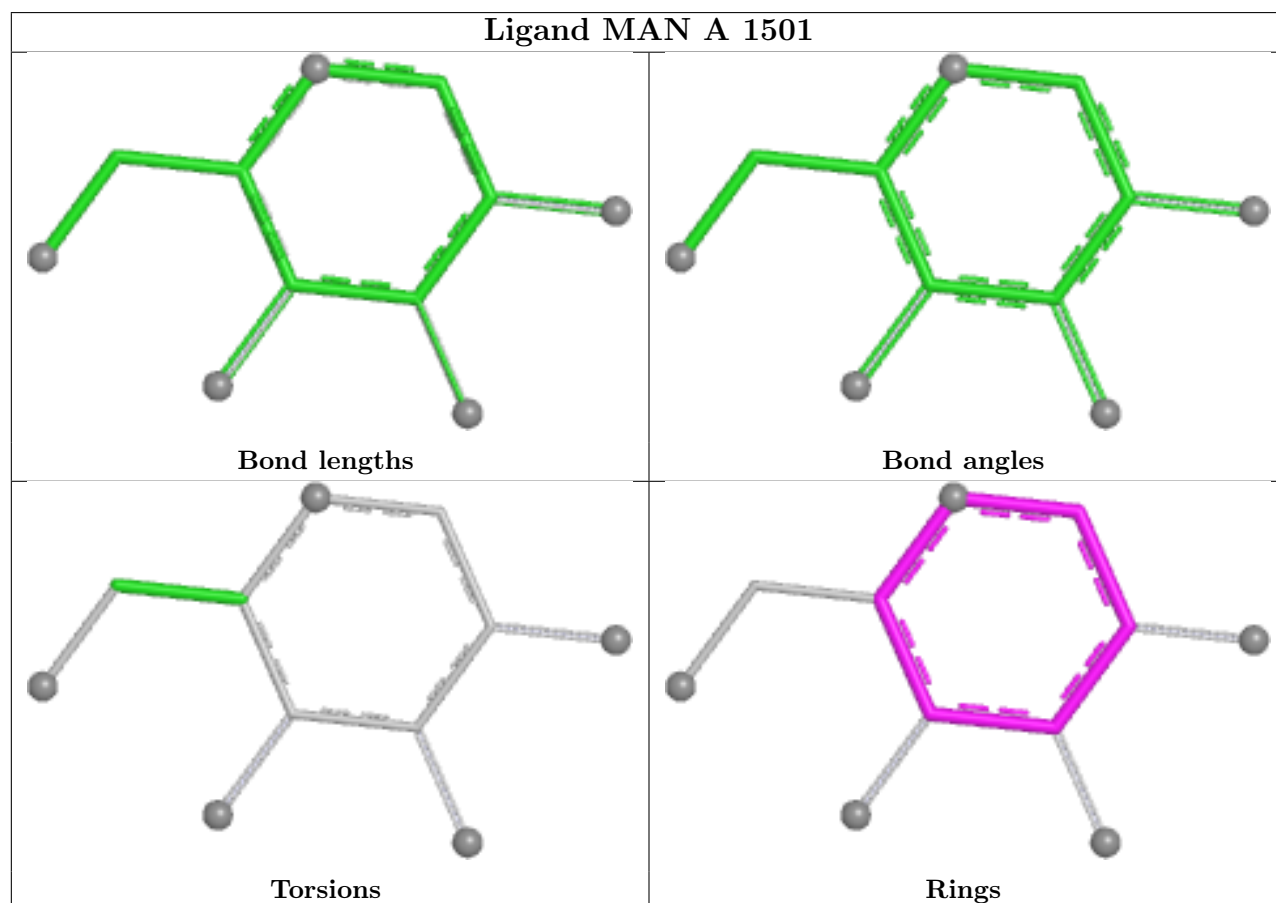
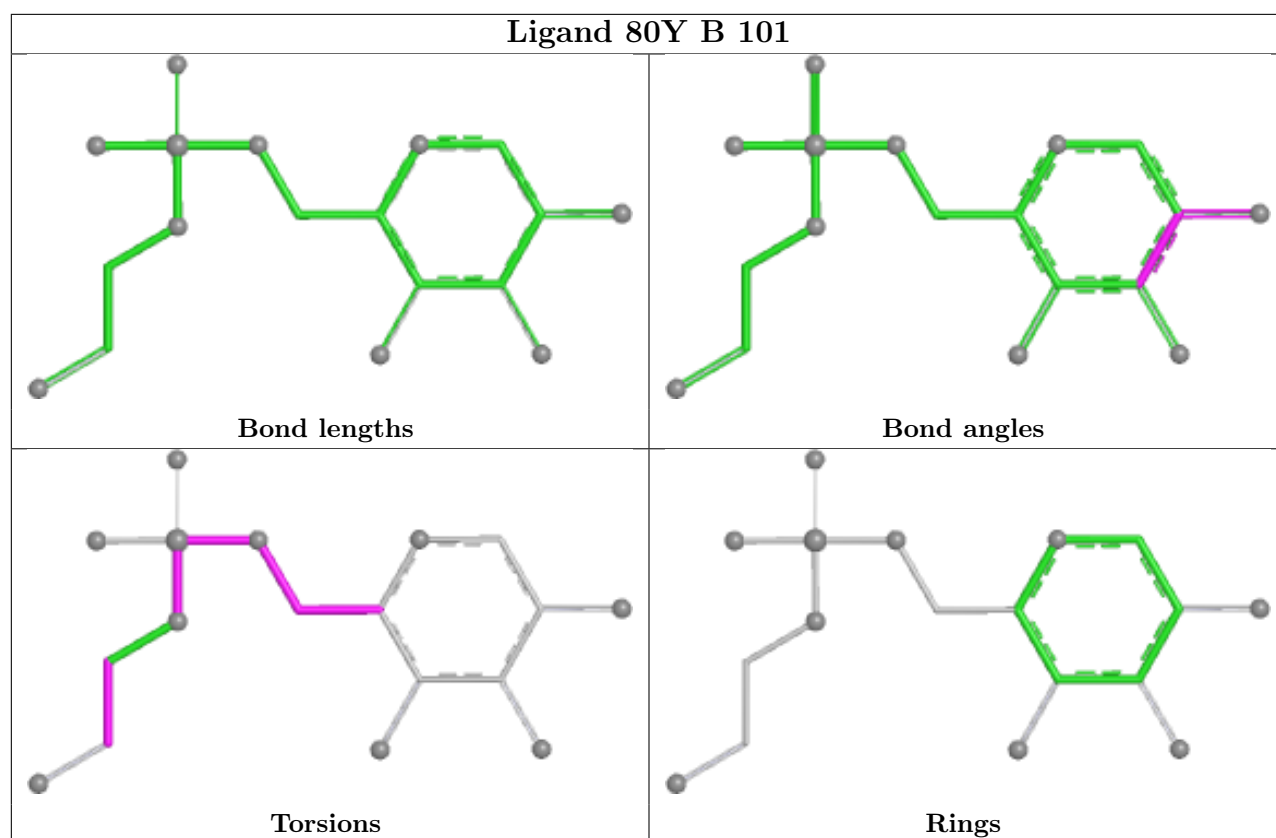
Mol	Chain	Res	Type	Atoms
3	A	1501	MAN	C1-C2-C3-C4-C5-O5

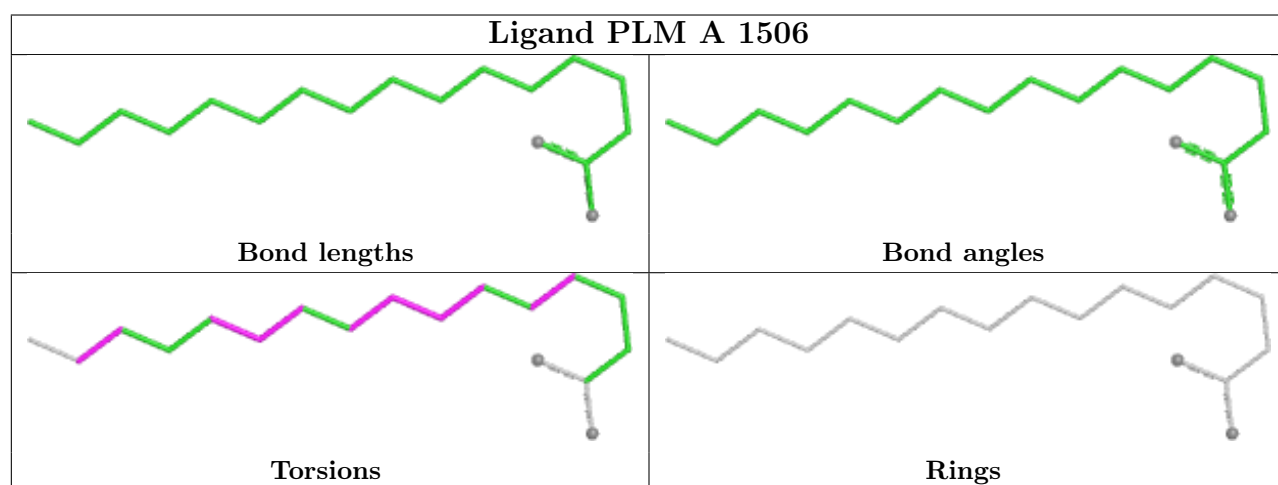
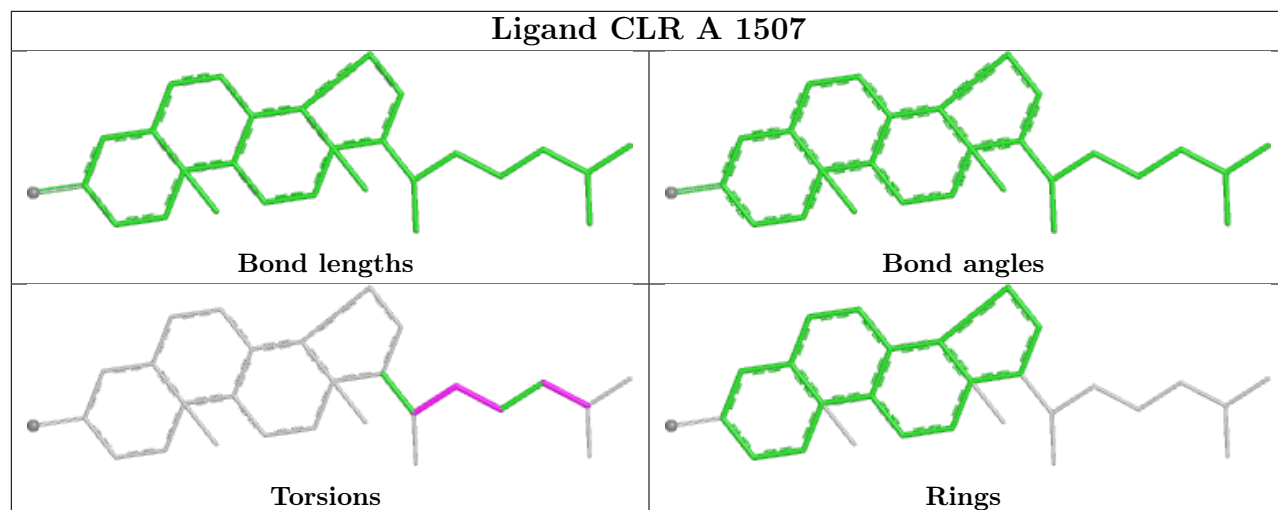
3 monomers are involved in 6 short contacts:

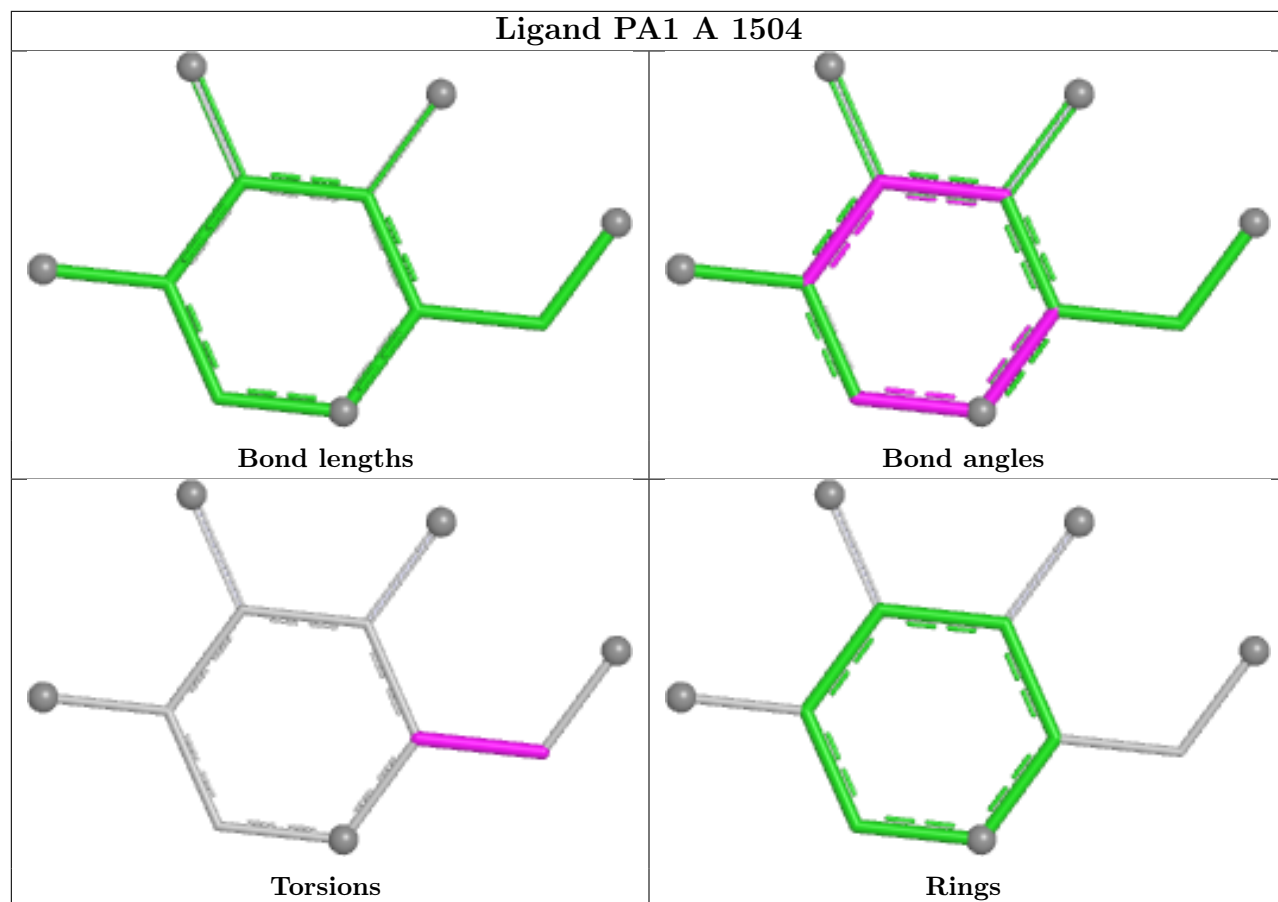
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1507	CLR	1	0
7	A	1506	PLM	4	0
5	A	1504	PA1	1	0

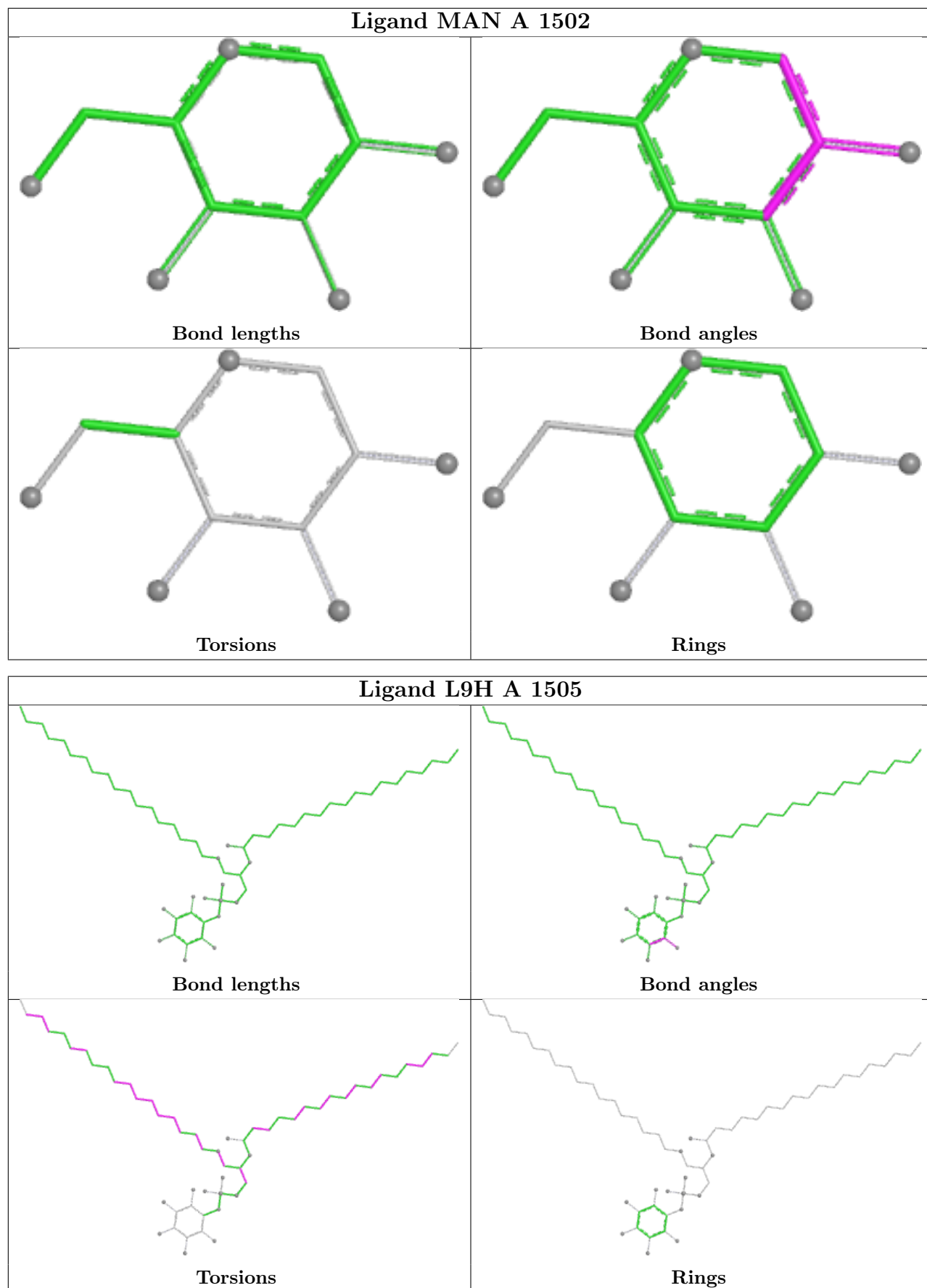
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

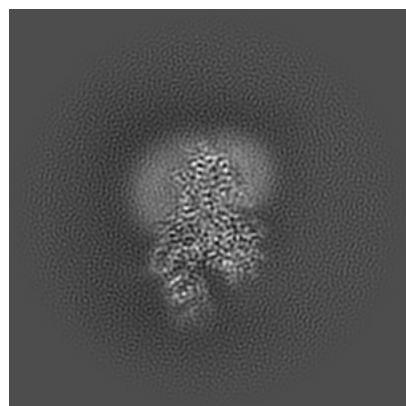
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36996. These allow visual inspection of the internal detail of the map and identification of artifacts.

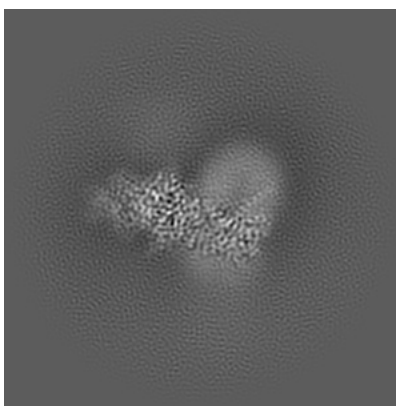
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

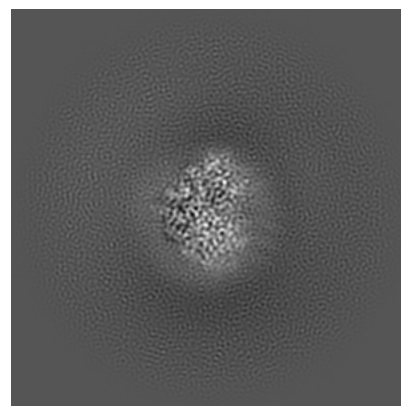
6.1.1 Primary map



X

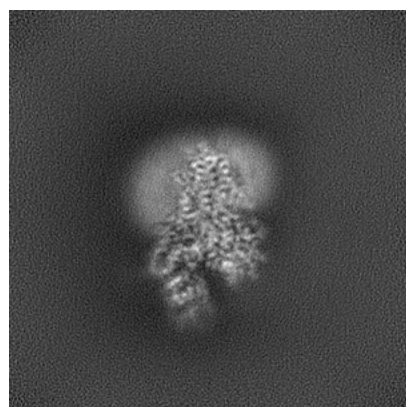


Y

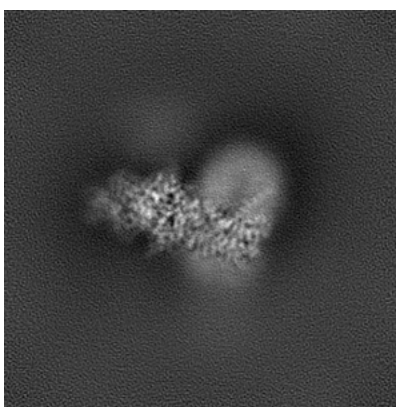


Z

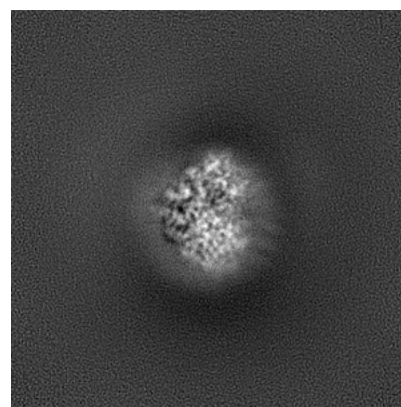
6.1.2 Raw map



X



Y

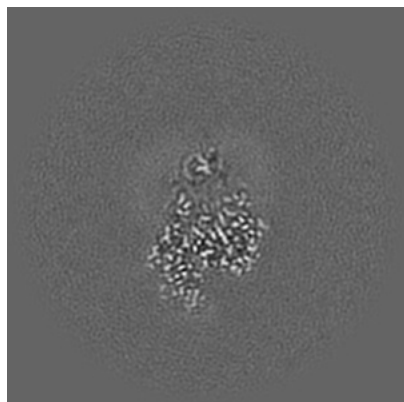


Z

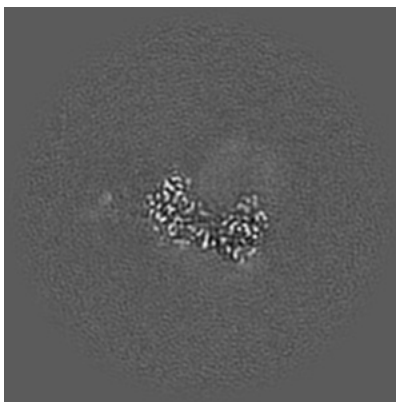
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

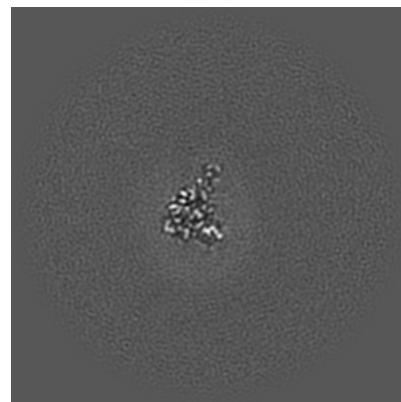
6.2.1 Primary map



X Index: 135

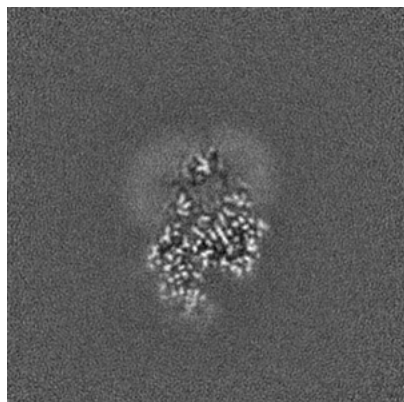


Y Index: 135

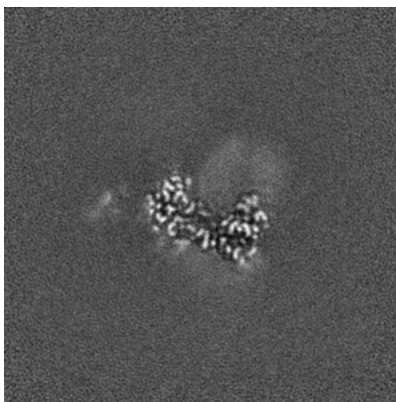


Z Index: 135

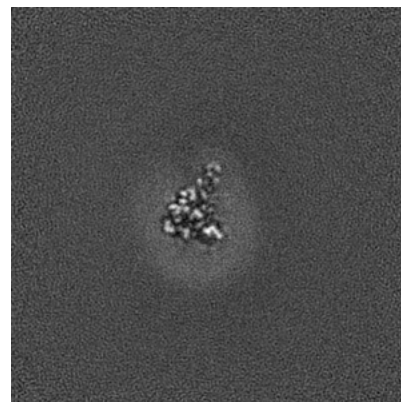
6.2.2 Raw map



X Index: 135



Y Index: 135

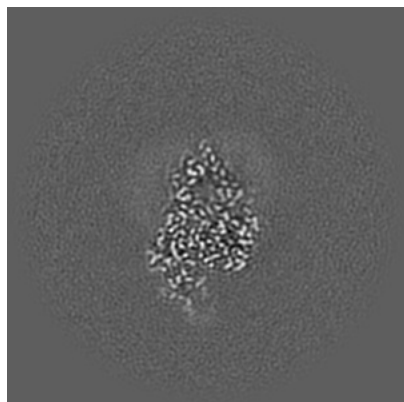


Z Index: 135

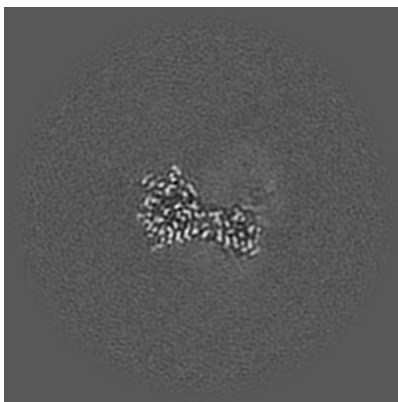
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

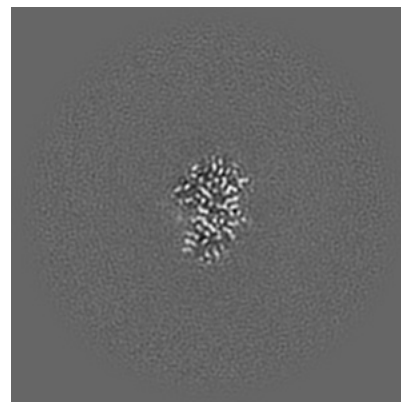
6.3.1 Primary map



X Index: 131

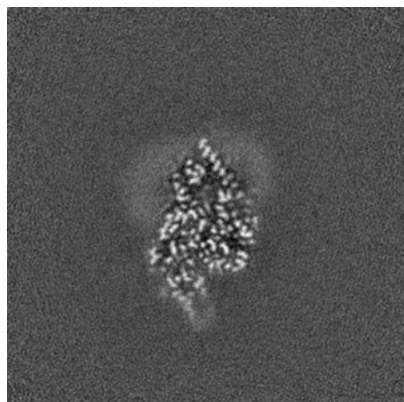


Y Index: 144

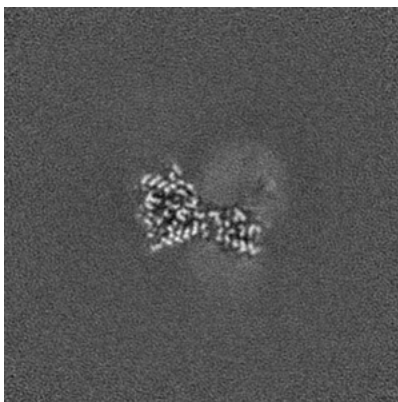


Z Index: 109

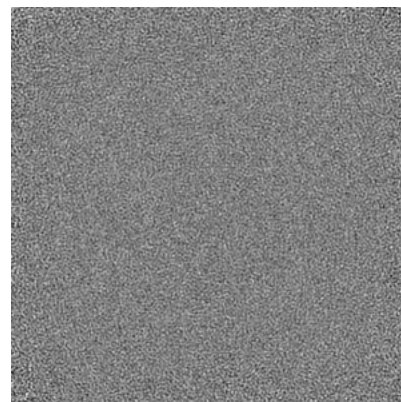
6.3.2 Raw map



X Index: 130



Y Index: 145

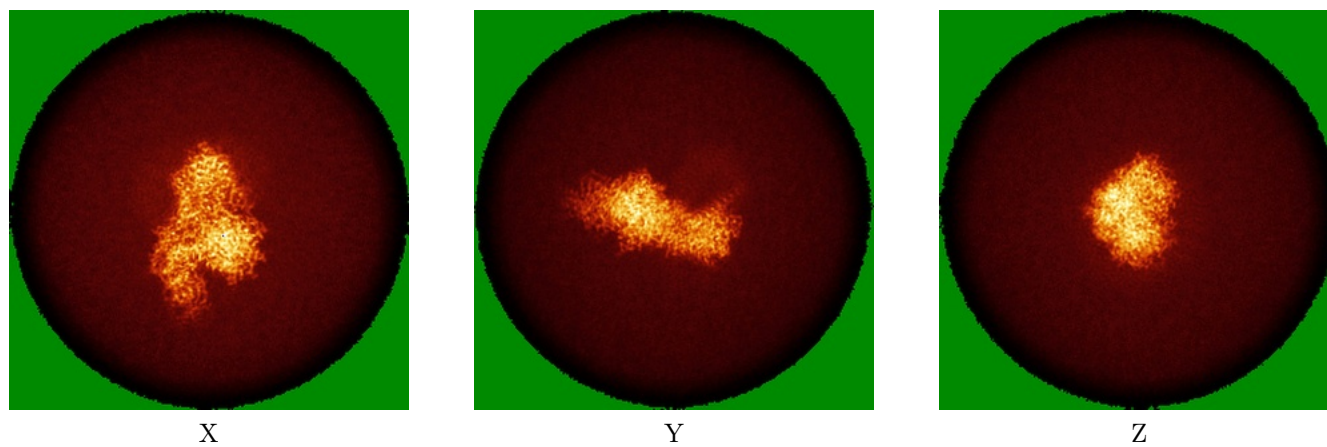


Z Index: 269

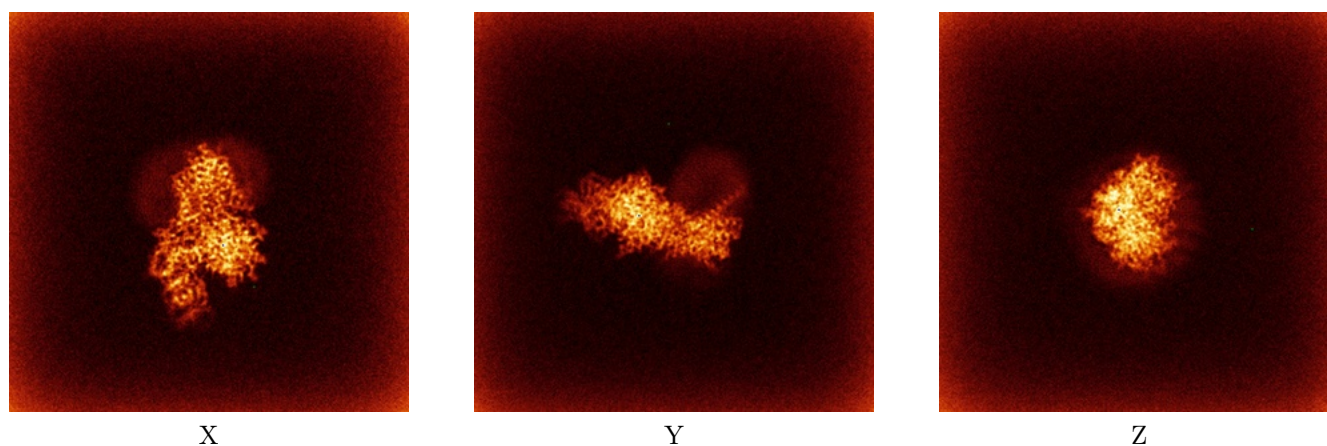
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

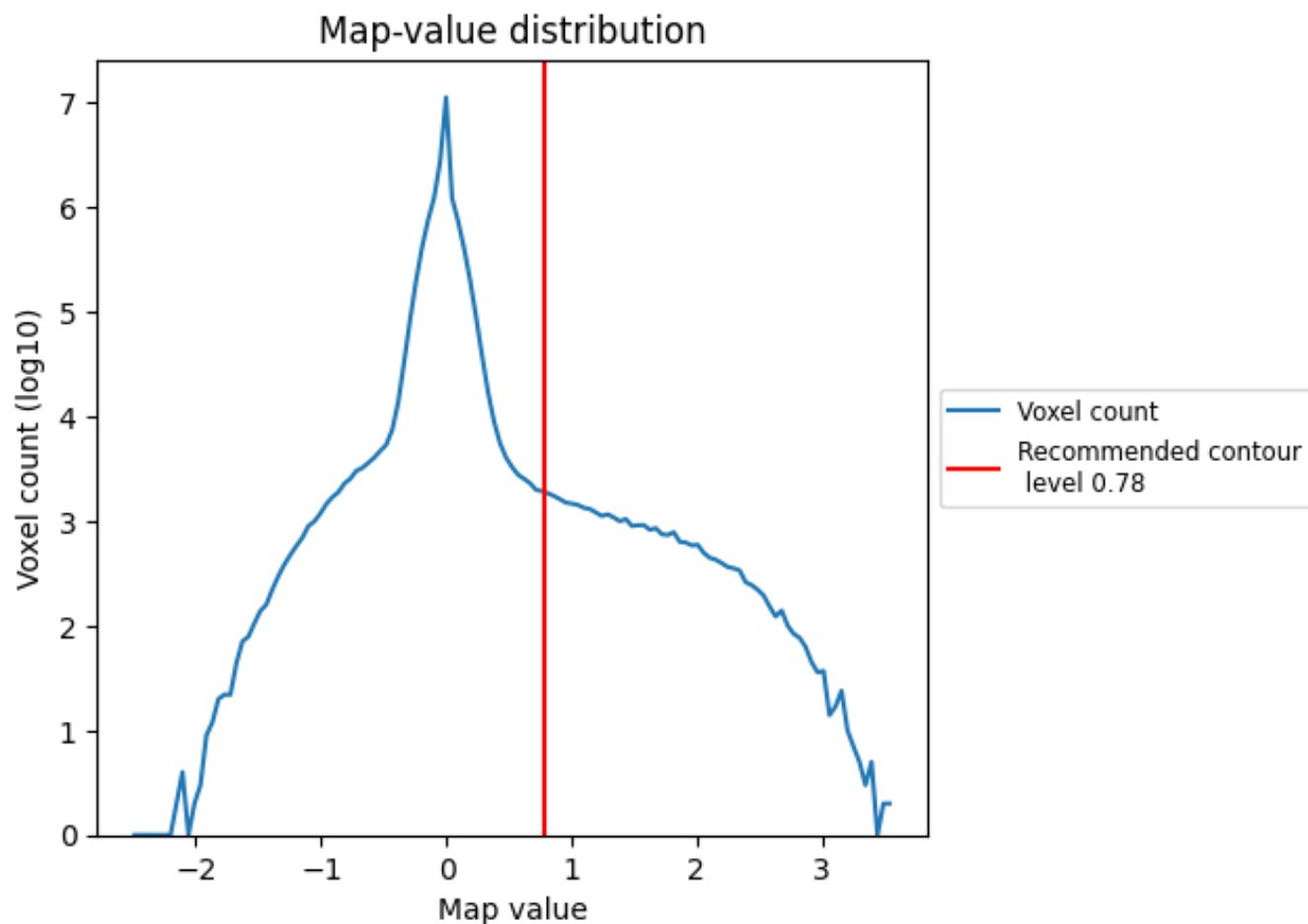
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

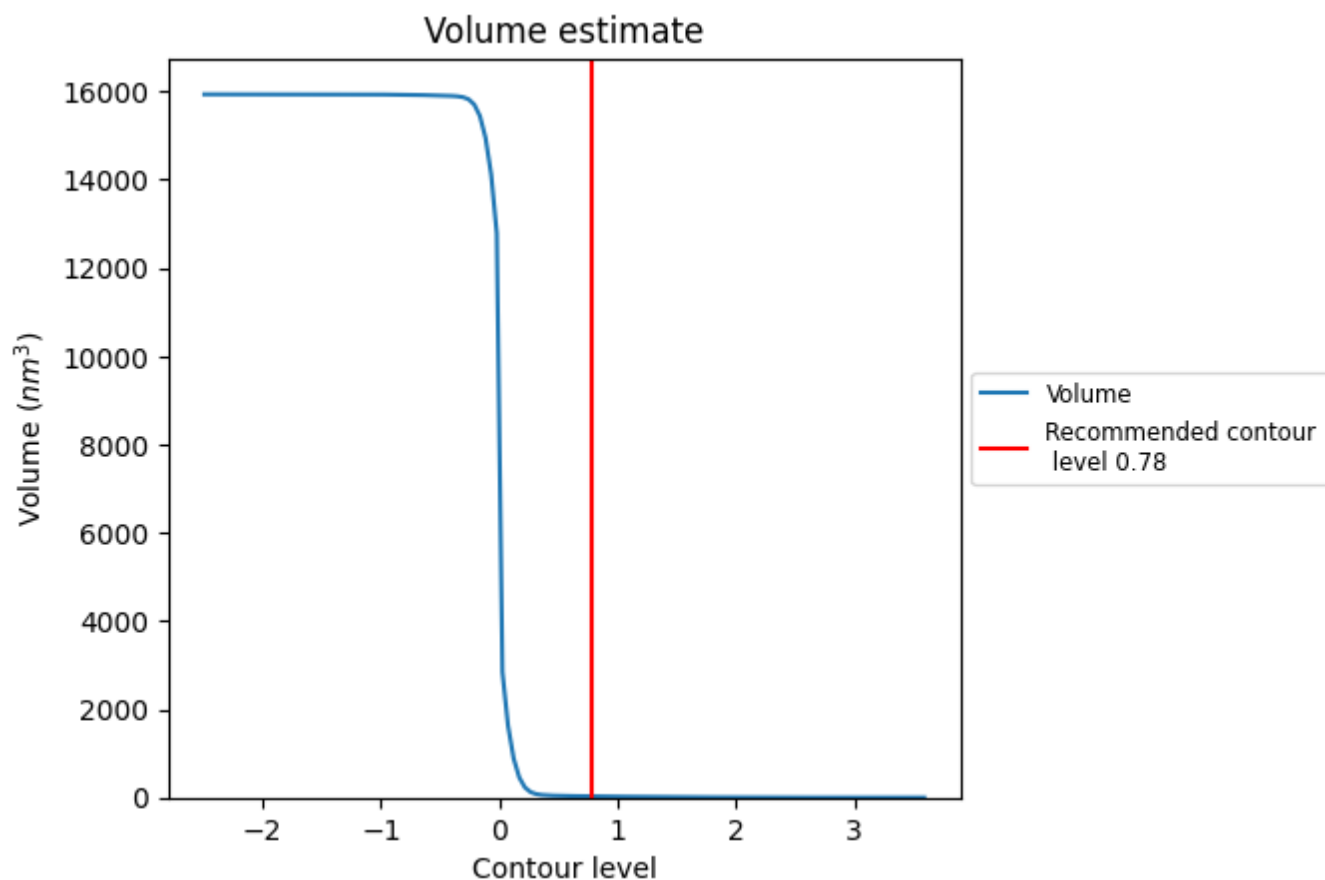
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

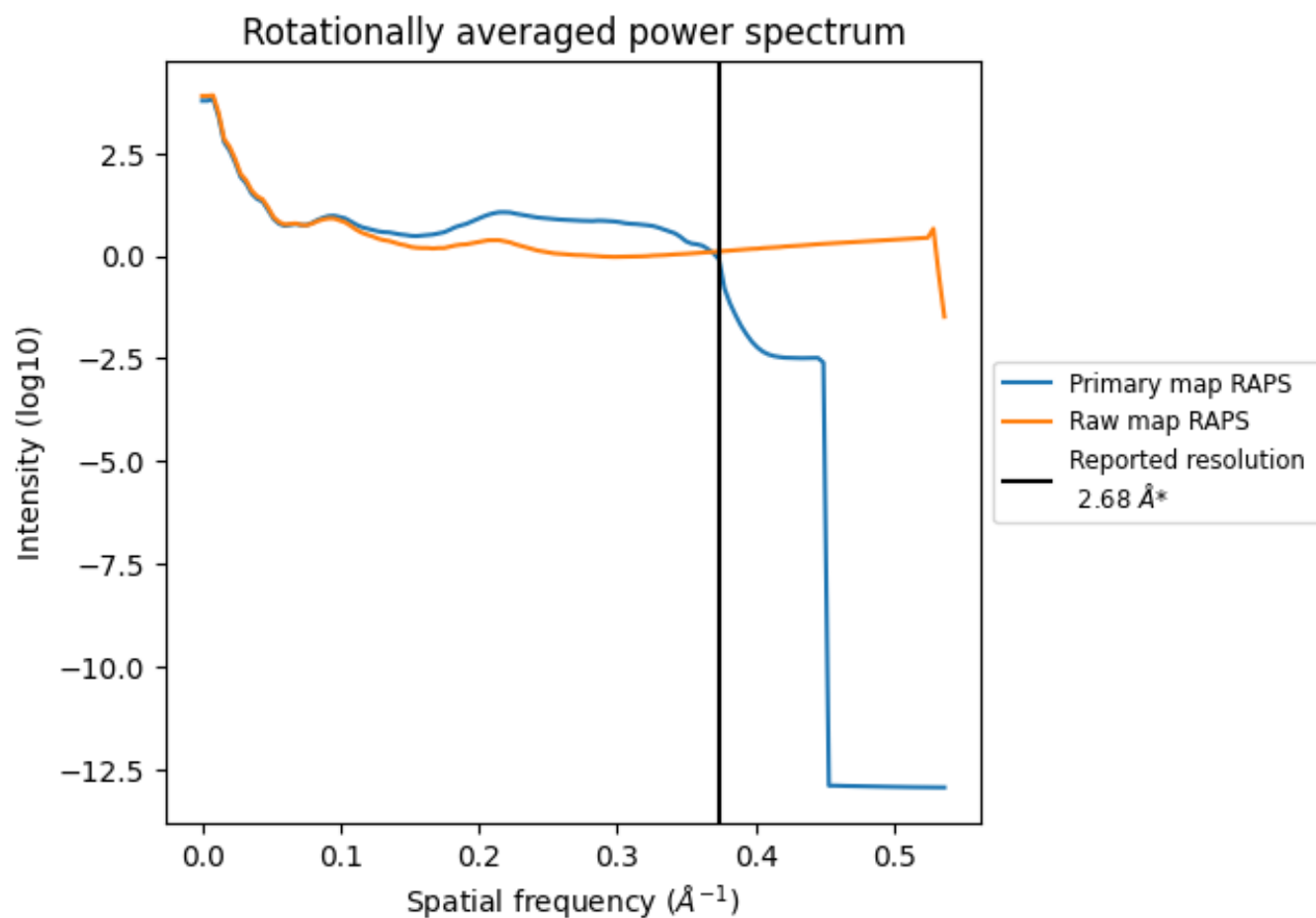
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 28 nm³; this corresponds to an approximate mass of 25 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

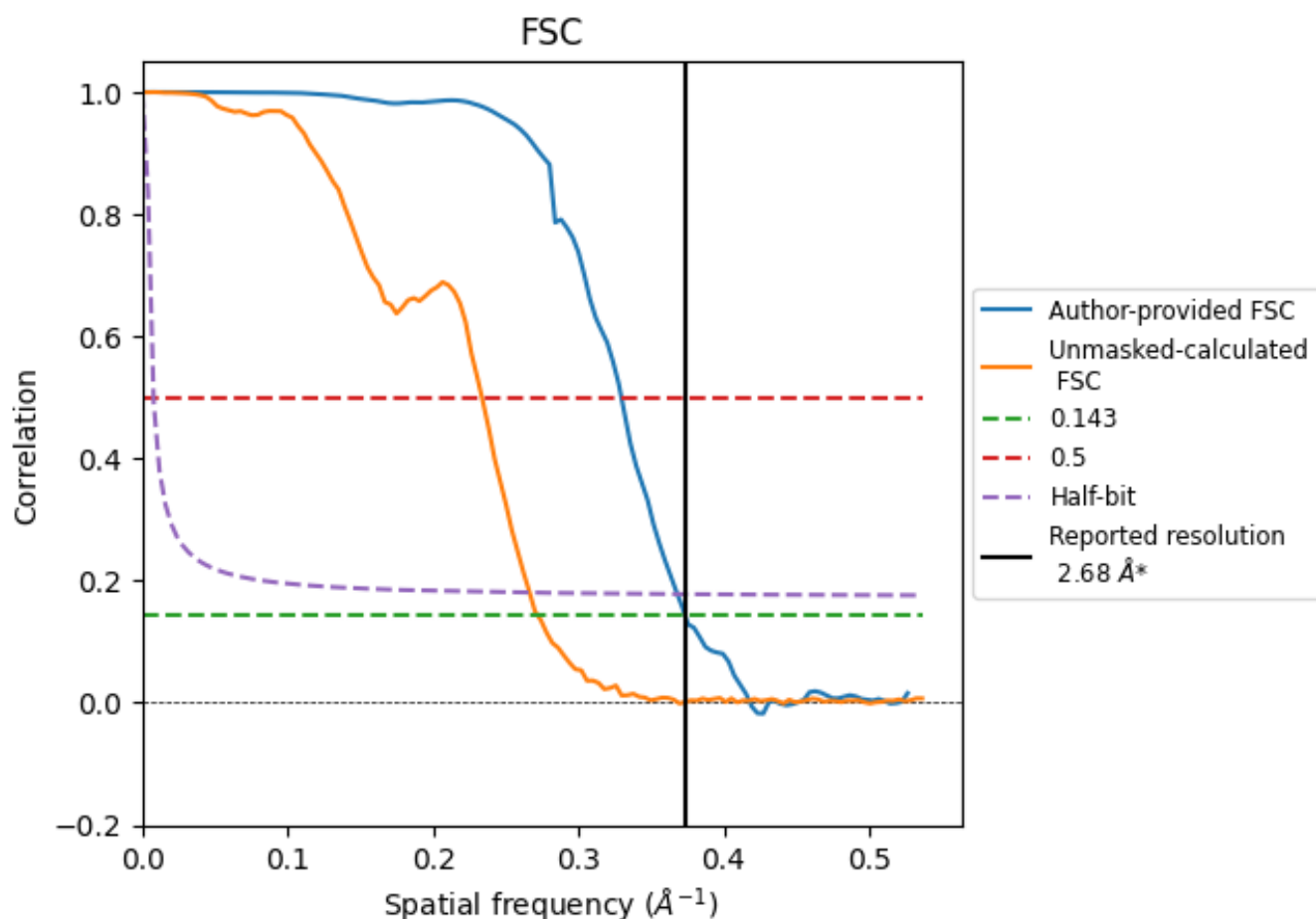


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.03	2.72
Unmasked-calculated*	3.68	4.28	3.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.68 differs from the reported value 2.68 by more than 10 %

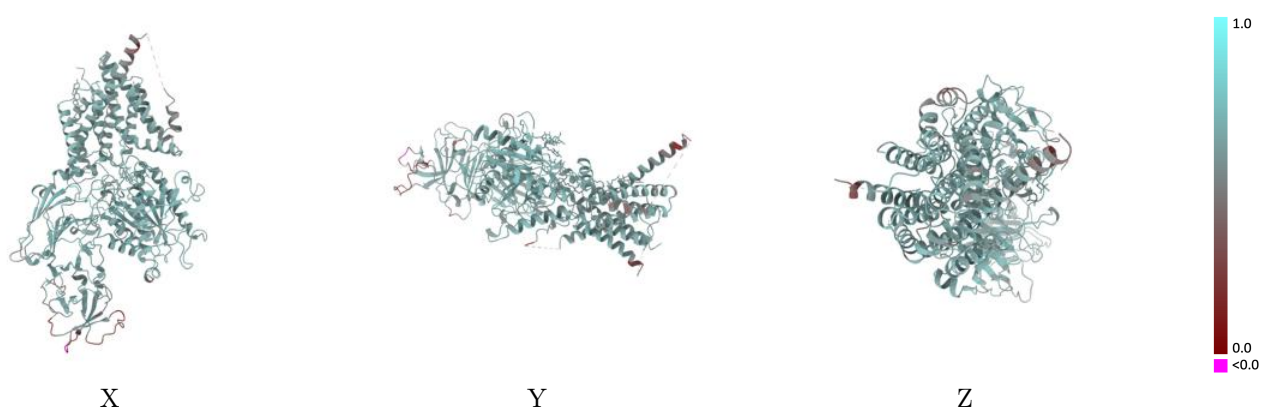
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-36996 and PDB model 8K9R. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

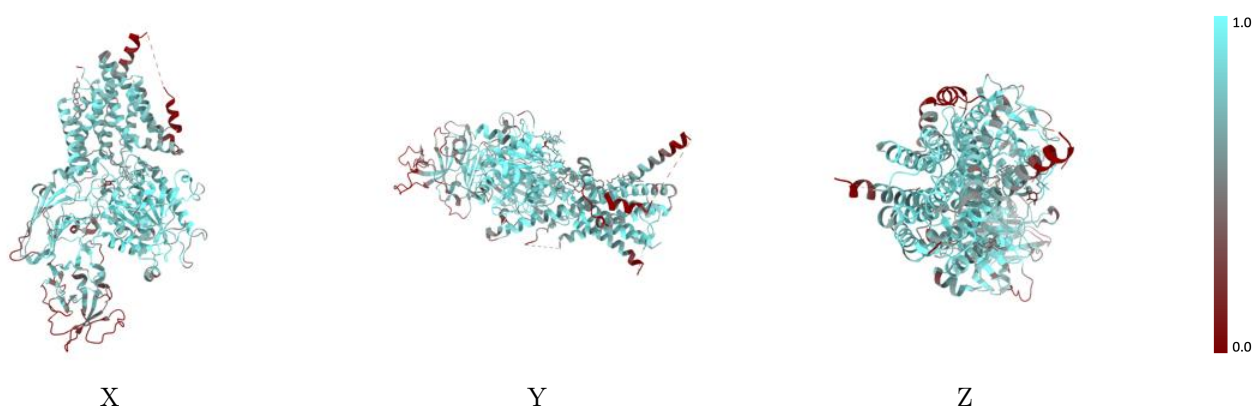
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



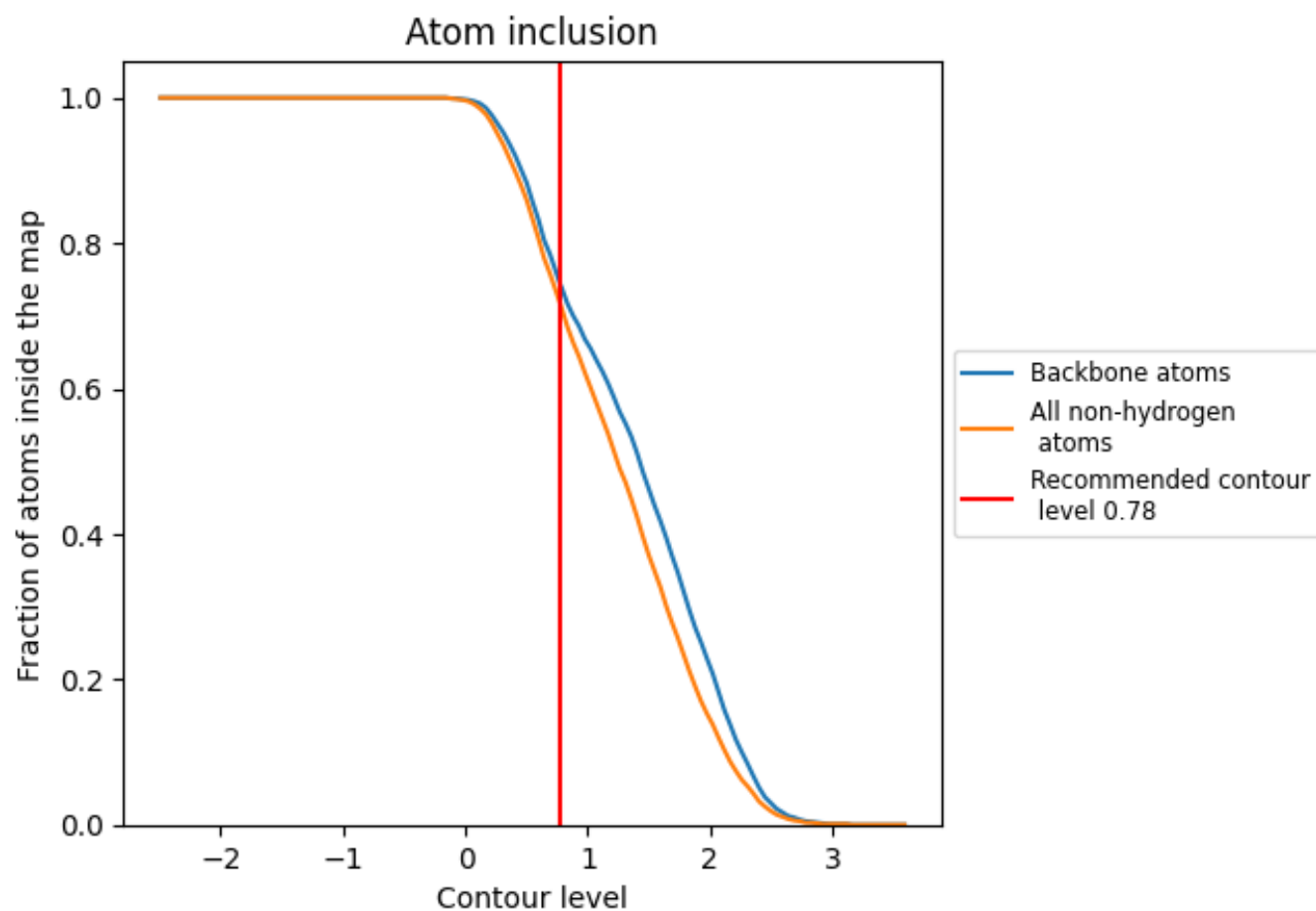
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.78).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.78) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.6040
A	0.7140	0.6040
B	0.6910	0.6060

